

SPECTRAL GAPS OF DIRAC OPERATORS WITH BOUNDARY CONDITIONS RELEVANT FOR GRAPHENE

RAFAEL D. BENGURIA, SØREN FOURNAIS, EDGARDO STOCKMEYER,
AND HANNE VAN DEN BOSCH

ABSTRACT. The two-dimensional Dirac operator describes low-energy excitations in graphene. Different boundary conditions correspond to different cuts of graphene samples, the most prominent being the so-called zigzag, armchair, and infinite mass conditions. We prove a lower bound to the spectral gap around zero, proportional to $|\Omega|^{-1/2}$, for Dirac operators in a domain Ω with various boundary conditions including the infinite mass and armchair cases. This bound does not apply to the zigzag realization which is known to be gapless. For the sake of completeness, we also provide a simple proof of the self-adjointness of these operators.

CONTENTS

1. Introduction	1
2. Self-adjointness	4
3. Lower bound for simply connected domains	11
Appendix A. Application to the two-valley description of graphene	15
Appendix B. Construction of a Weyl sequence	16
References	17

1. INTRODUCTION

Graphene is a two-dimensional sheet of carbon atoms forming a honeycomb lattice. It is well-known that low-energy electronic excitations in graphene can be described as Dirac fermions (see [9] for a review). In its most elementary form, a quasi-particle with momentum close to a so-called Dirac point, can be described by a two-spinor. Each of its components represents the occupation of one of the two triangular sublattices that form the honeycomb structure. The energy of the quasi-particle is given by the Dirac operator

$$T = v_f \hbar (-i \boldsymbol{\sigma} \cdot \nabla),$$

where $v_f \sim 10^6 \text{m/s}$ is the Fermi velocity. In order to take into account contributions from the two inequivalent Dirac points (valleys), one needs two copies of this operator acting on a four-component spinor.

If the piece of graphene has a boundary, the question arises which boundary conditions to impose. On physical grounds, one expects the boundary condition to be local. In this case, it can be written, in each point, as a two-dimensional projection in \mathbb{C}^4 . A detailed treatment of the possible boundary conditions for

straight edges can be found in [2]. In the physics literature the so-called zigzag, armchair and infinite mass boundary conditions are the most commonly used.

For simplicity we will restrict ourselves to \mathbb{C}^2 -spinors for most of this work and translate our results to the \mathbb{C}^4 -case in Appendix A. In this case, requiring the Dirac operator to be symmetric reduces the possible boundary conditions to a one-parameter family. Mathematically, this problem has first been addressed in [5], as an example of a chaotic system with time-reversal symmetry breaking. In [17] it was shown that zero is an eigenvalue of infinite multiplicity of the zigzag operator. This was further explored in [11] for certain perturbed zigzag operators. In [18] it was shown that the infinite mass operator can be obtained as a limit of Dirac operators with a mass term supported outside the domain under consideration.

Here we study which boundary conditions make the Dirac operator self-adjoint on a domain contained in the first Sobolev space $H^1(\Omega, \mathbb{C}^2)$, where Ω is the domain under consideration. For a smaller class of boundary conditions, including armchair and infinite mass, we prove that zero is never in the spectrum of the corresponding operator. In this case, we obtain an explicit lower bound for the distance of the spectrum to zero. This contrasts with the spectrum for zigzag boundaries. In fact, this difference may be detected experimentally, see e.g. [15].

1.1. Definitions and results. We consider a two-dimensional Dirac operator on a bounded domain $\Omega \subset \mathbb{R}^2$ with C^2 -boundary $\partial\Omega$. Choosing appropriate units, the Dirac operator acts as the differential expression

$$T \equiv -i\boldsymbol{\sigma} \cdot \nabla = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (-i\partial_1) + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} (-i\partial_2).$$

We will write D_η for the operator acting as T on functions in the domain

$$\mathcal{D}(D_\eta) \equiv \{u \in H^1(\Omega, \mathbb{C}^2) \mid P_{-, \eta} \gamma u = 0\}.$$

Here γ is the trace operator on the boundary of Ω and the orthogonal projections $P_{\pm, \eta}$ are defined as

$$P_{\pm, \eta} = 1/2(1 \pm A_\eta), \quad A_\eta = \cos(\eta)\boldsymbol{\sigma} \cdot \boldsymbol{t} + \sin(\eta)\sigma_3,$$

where \boldsymbol{t} is the unit vector tangent to the boundary. A priori, η can be any real function of $\partial\Omega$, but in the physically relevant cases it is a constant on each connected component of $\partial\Omega$. The boundary conditions with $\cos \eta = 0$ are called *zigzag* boundary conditions, while the ones with $\cos \eta = \pm 1$ are referred to as *infinite mass* boundary conditions.

Using integration by parts and the hermiticity of the Pauli matrices, it is straightforward to check that in this domain D_η is a symmetric operator. For all $u, v \in H^1(\Omega, \mathbb{C}^2)$,

$$\begin{aligned} \langle u, Tv \rangle &= \int_{\Omega} -i (u, \boldsymbol{\sigma} \cdot \nabla v)_{\mathbb{C}^2} \\ (1) \quad &= \int_{\Omega} -i \cdot \nabla (u, \boldsymbol{\sigma} v)_{\mathbb{C}^2} + i \int_{\Omega} (\boldsymbol{\sigma} \cdot \nabla u, v)_{\mathbb{C}^2} \\ &= \langle Tu, v \rangle - i \int_{\partial\Omega} (u, \boldsymbol{n} \cdot \boldsymbol{\sigma} v)_{\mathbb{C}^2}, \end{aligned}$$

where \boldsymbol{n} is the outward normal vector to $\partial\Omega$. If $u, v \in \mathcal{D}(D_\eta)$, the boundary term cancels since the anticommutator $\{A_\eta, \boldsymbol{n} \cdot \boldsymbol{\sigma}\} = 0$.

Remark 1. From the previous calculation (1) we see that for all $u \in C_0^\infty$ we have

$$(2) \quad \|Tu\|^2 = \langle u, T^2u \rangle = \langle u, -\Delta u \rangle = \|\nabla u\|^2.$$

To determine when D_η is actually self-adjoint, in the case of C^∞ -boundaries, one may adapt the corresponding theorems of [6] to our case (see for instance [16]). However, the operators treated in [6] are more general and the proofs require sophisticated techniques from the analysis of pseudodifferential operators. Our proof, given in Section 2, is simpler and it works for C^2 -boundaries as well. We have,

Theorem 1.1. *Given $\Omega \subset \mathbb{R}^2$, bounded, with C^2 -boundary, and $\eta \in C^1(\partial\Omega)$, define D_η as above. If $\cos \eta(s) \neq 0$ for all $s \in \partial\Omega$, then D_η is self-adjoint on $\mathcal{D}(D_\eta)$.*

Remark 2. Our proof of self-adjointness is really an elliptic regularity result for the Dirac system. We implicitly establish the following inequality:

Suppose that Ω and η satisfy the conditions of Theorem 1.1. Then there exists a constant $C > 0$ such that

$$(3) \quad \|u\|_{H^1(\Omega)} \leq C (\|u\|_{L^2(\Omega)} + \|Tu\|_{L^2(\Omega)}),$$

for all $u \in L^2(\Omega, \mathbb{C}^2)$ satisfying the boundary condition $P_{-, \eta} \gamma u = 0$. Notice that we establish below that the boundary trace γu exists in $H^{-1/2}(\partial\Omega)$ if $u, Tu \in L^2(\Omega, \mathbb{C}^2)$.

If D_η is self-adjoint on a domain contained in $H^1(\Omega, \mathbb{C}^2)$, it follows from the compact embedding of $H^1(\Omega) \subset L^2(\Omega)$ that its resolvent is compact. Thus, the spectrum of D_η consists of eigenvalues of finite multiplicity accumulating only at $\pm\infty$.

This is to be contrasted with the case $\cos \eta = 0$ where zero is an eigenvalue of infinite multiplicity of D_η , showing that the operator cannot be self-adjoint on a subset of $H^1(\Omega, \mathbb{C}^2)$. For non-constant η such that $\cos \eta(s)$ tends to zero at least quadratically when $s \rightarrow s_0 \in \partial\Omega$, we can still show $0 \in \sigma_{\text{ess}}(D_\eta)$ (see Appendix B for a precise statement and proof of this point). On the other hand, for constant η and simply connected domains, we obtain the following lower bound for the spectral gap whose proof can be found in Section 3.

Theorem 1.2. *Take $\Omega \subset \mathbb{R}^2$ simply connected with C^2 -boundary, $\eta \neq \pm\pi/2$ a constant and D_η as before. Set $B = \min(|\cos \eta/(1 - \sin \eta)|, |(1 - \sin \eta)/\cos \eta|)$. If λ is an eigenvalue of D_η , then*

$$\lambda^2 \geq \frac{2\pi}{|\Omega|} B^2.$$

Remark 3. The bound is not sharp, but it is quite good, as a comparison with the case of a disc shows. When $\eta \equiv 0$, the lowest eigenvalue for a disc of unit radius is k_0 , the smallest positive number such that $J_0(k_0) = J_1(k_0)$, where J_n is the n -th Bessel function of the first kind (see [5]). Numerically, $k_0 \approx 1.435$, and our lower bound reads

$$k_0 > \sqrt{2} \approx 1.414.$$

Remark 4. In physical units our lower bound for armchair or infinite mass boundary conditions (see Appendix A) gives a gap larger than $2\sqrt{2\pi\hbar v_f}|\Omega|^{-1/2}$. This means that in order to obtain a gap of 1 eV one needs a domain of about 10 nm of diameter.

In the differential geometry literature, much attention has been devoted to lower bounds for the square of Dirac operators on surfaces. Most of these results deal with closed surfaces [12, 4]. For Dirac operators on two-dimensional manifolds with boundaries a less explicit bound has been derived in [13]. Our proof uses ideas from [4].

1.2. Notation. Before going further, we need to fix some notations. Vectors in \mathbb{R}^2 will be written in boldface and the scalar product between $\mathbf{r}_1, \mathbf{r}_2$ is written $\mathbf{r}_1 \cdot \mathbf{r}_2$. An asterisk means either the conjugate of a complex number or the adjoint of an operator. For spinor fields, $(\cdot, \cdot)_{\mathbb{C}^2}$ will denote the scalar product in \mathbb{C}^2 and $\langle \cdot, \cdot \rangle_A$ will be used for the scalar product in $L^2(A, \mathbb{C}^2)$. When the domain of definition is clear from the context, we will write $\langle \cdot, \cdot \rangle$. The norms in the Sobolev space $H^s(A, \mathbb{C}^2)$ will be denoted by $\|\cdot\|_{H^s}$ when the domain of definition is clear from the context. When there is no ambiguity, we also write $\|\cdot\|_{L^2} = \|\cdot\|$.

We will consider a fixed domain Ω with C^2 -boundary $\partial\Omega$. We denote by $\mathbf{n}(s)$ and $\mathbf{t}(s)$ the outward normal and the tangent vector to the boundary at the point $s \in \partial\Omega$. The orientation of \mathbf{t} is chosen such that \mathbf{n}, \mathbf{t} is positively oriented, so we have $\mathbf{t} \cdot \nabla \mathbf{t}(s) := \partial_t \mathbf{t}(s) = -\kappa(s)\mathbf{n}(s)$, where $\kappa(s)$ is the curvature of the boundary. If $\mathbf{t}(s) = (t_1(s), t_2(s))$, we define $t(s) = t_1(s) + it_2(s)$, the tangent vector seen as a number in \mathbb{C} . Associated to the domain Ω we have the trace operator at the boundary $\gamma : C^1(\overline{\Omega}) \rightarrow C^1(\partial\Omega)$, and an extension operator $E : C^1(\partial\Omega) \rightarrow C^1(\overline{\Omega})$. We recall that γ extends to a bounded operator from $H^{s+1/2}(\Omega)$ to $H^s(\partial\Omega)$, and E from $H^s(\partial\Omega)$ to $H^{s+1/2}(\Omega)$ for all $s \in (0, 2)$.

In passing, we also recall our definition for the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

They satisfy the (anti)commutation relations

$$\{\sigma_j, \sigma_k\} = 2\delta_{jk}, \quad [\sigma_j, \sigma_k] = 2i\epsilon_{jkl}\sigma_l, \quad j, k, l \in \{1, 2, 3\},$$

where δ_{jk} is the Kronecker delta and ϵ_{jkl} is the Levi-Civita symbol, which is totally antisymmetric and normalized by $\epsilon_{123} = 1$.

For an open set Ω we denote by $\mathcal{D}'(\Omega)$ the space of distributions, i.e., the dual of $C_0^\infty(\Omega)$.

2. SELF-ADJOINTNESS

The goal here is to prove Theorem 1.1. In order to keep notations simple, we will consider a fixed C^1 -function η and suppress the dependence on η from the notations.

2.1. General considerations. First, we will need some regularity properties of $v \in \mathcal{D}(D^*)$.

Lemma 2.1. *Let $\mathcal{K} := \{u \in L^2(\Omega, \mathbb{C}^2) \mid Tu \in L^2(\Omega, \mathbb{C}^2)\}$ equipped with the graph-norm $\|u\|_{\mathcal{K}}^2 = \|u\|^2 + \|Tu\|^2$, where T acts as a differential operator on distributions in Ω . Then \mathcal{K} is a Hilbert space and $C^\infty(\overline{\Omega}, \mathbb{C}^2)$ is dense in \mathcal{K} .*

Proof. First we show that \mathcal{K} is a Hilbert space. Take a Cauchy sequence $(u_n)_{n \in \mathbb{N}} \subset \mathcal{K}$ with $u_n \rightarrow u$ and $Tu_n \rightarrow v$ in L^2 . We have for any test function $\varphi \in C_0^\infty(\Omega)$

$$Tu[\varphi] = u[T\varphi] = \lim_{n \rightarrow \infty} \langle u_n, T\varphi \rangle = \lim_{n \rightarrow \infty} Tu_n[\varphi] = \lim_{n \rightarrow \infty} \langle Tu_n, \varphi \rangle = \langle v, \varphi \rangle.$$

Therefore, $Tu = v$ and in particular $u \in \mathcal{K}$.

Recall that by definition $u \in C^\infty(\overline{\Omega})$ iff u is the restriction to Ω of a smooth function (spinor) on \mathbb{R}^2 . To prove the density of $C^\infty(\overline{\Omega})$ it suffices to show that if

$$(4) \quad \langle v, u \rangle_{\mathcal{K}} = \langle v, u \rangle + \langle Tv, Tu \rangle = 0,$$

for all $u \in C^\infty(\overline{\Omega})$ then v vanishes. Let $w := Tv \in L^2(\Omega)$. It follows from (4) that

$$(5) \quad Tw = -v \quad \text{in } \mathcal{D}'(\Omega).$$

Define \tilde{v} and \tilde{w} as the extensions by zero to $L^2(\mathbb{R}^2)$ of v and w , respectively. For any $\varphi \in C_0^\infty(\mathbb{R}^2)$ we calculate using (4)

$$T\tilde{w}[\varphi] = \langle \tilde{w}, T\varphi \rangle_{L^2(\mathbb{R}^2)} = \langle w, T\varphi \rangle_{L^2(\Omega)} = \langle -v, \varphi \rangle_{L^2(\Omega)} = \langle -\tilde{v}, \varphi \rangle_{L^2(\mathbb{R}^2)}.$$

Therefore, $T\tilde{w} = -\tilde{v} \in L^2(\mathbb{R}^2)$. By ellipticity we find that $\tilde{w} \in H^1(\mathbb{R}^2)$. Moreover, using [8, Proposition IX.18] we get that $w \in H_0^1(\Omega)$.

Let $(\varphi_n)_{n \in \mathbb{N}} \subset C_0^\infty(\Omega)$ be a sequence with $\varphi_n \rightarrow w$ in $H^1(\Omega)$. For any $u \in \mathcal{K}$

$$\begin{aligned} \langle v, u \rangle_{\mathcal{K}} &= \langle v, u \rangle_{L^2(\Omega)} + \langle w, Tu \rangle_{L^2(\Omega)} \\ &= \langle v, u \rangle_{L^2(\Omega)} + \lim_{n \rightarrow \infty} \langle T\varphi_n, u \rangle_{L^2(\Omega)} \\ &= \langle v, u \rangle_{L^2(\Omega)} + \langle Tw, u \rangle_{L^2(\Omega)} = 0, \end{aligned}$$

where the last equality follows from (5) and implies that $v = 0$. \square

Lemma 2.2. *We have that $\mathcal{D}(D^*) \subset \mathcal{K}$. Moreover, $\mathcal{K} \subset H_{\text{loc}}^1(\Omega, \mathbb{C}^2)$.*

Proof. Fix $v \in \mathcal{D}(D^*)$ and define $\tilde{v} := D^*v \in L^2(\Omega)$. By definition Tv is a distribution, thus for any $u \in C_0^\infty(\Omega)$

$$Tv[u] \equiv \langle v, Tu \rangle = \langle v, Du \rangle = \langle \tilde{v}, u \rangle,$$

since $C_0^\infty(\Omega) \subset \mathcal{D}(D)$. This shows that the distribution Tv can be identified with the L^2 -function D^*v and thus $v \in \mathcal{K}$.

Let now $v \in \mathcal{K}$. By Lemma 2.1 we may choose a sequence of $C^\infty(\Omega)$ -functions $(v_n)_{n \in \mathbb{N}}$ that converges to v in $L^2(\Omega)$ and such that Tv_n converges to Tv in $L^2(\Omega)$.

Fix an open set A such that $\bar{A} \subset \Omega$. We will show that ∇v_n converges in $L^2(A)$. Take a cut-off function $\chi_A \in C_0^\infty(\Omega)$ such that $\chi_A = 1$ on A . Now we can use (2) to show that ∇v_n is a Cauchy sequence

$$\begin{aligned} \int_A |\nabla(v_n - v_m)|_{\mathbb{C}^2}^2 &\leq \int_\Omega |\nabla \chi_A(v_n - v_m)|_{\mathbb{C}^2}^2 \\ &= \int_\Omega |T\chi_A(v_n - v_m)|_{\mathbb{C}^2}^2 \\ &\leq \|\nabla \chi_A\|_\infty^2 \|v_n - v_m\|^2 + \|T(v_n - v_m)\|^2. \end{aligned}$$

This finishes the proof. \square

By Lemma 2.2 the difficult part in proving the inclusion $\mathcal{D}(D^*) \subset \mathcal{D}(D)$ is to show regularity of $v \in \mathcal{D}(D^*)$ up to the boundary. To do so it is sufficient to prove that v has a sufficiently regular trace on the boundary $\partial\Omega$. First we show that traces exist as distributions.

Lemma 2.3. *The trace γ extends to a continuous map $\gamma : \mathcal{K} \rightarrow H^{-1/2}(\partial\Omega, \mathbb{C}^2)$. Moreover, if $v \in \mathcal{D}(D^*)$ then $P_- \gamma v = 0$. An equivalent formulation of this is that $\gamma v_2 = \frac{1 - \sin(\eta)}{\cos(\eta)} t \gamma v_1$.*

Proof. Let $v \in \mathcal{K}$ and let $(v_n)_{n \in \mathbb{N}}$ be a $C^\infty(\overline{\Omega})$ -sequence approximating v in the \mathcal{K} -norm. We will show that the traces γv_n of the v_n 's converge in $H^{-1/2}(\partial\Omega)$.

Fix $f \in C^\infty(\partial\Omega)$. By [1, Theorem 7.53] it is possible to extend f to a regular function $u \equiv Ef$ on Ω satisfying $\gamma u = f$ with $\|u\|_{H^1(\Omega)} \leq C_E \|f\|_{H^{1/2}(\partial\Omega)}$, with C_E only depending on Ω . By the same calculation as in (1),

$$i \int_{\partial\Omega} (\gamma v_n, \boldsymbol{\sigma} \cdot \mathbf{n} f) = \langle T v_n, u \rangle - \langle v_n, T u \rangle.$$

This shows

$$\begin{aligned} |\langle \gamma(v_n - v_m), \boldsymbol{\sigma} \cdot \mathbf{n} f \rangle_{\partial\Omega}| &\leq \|T(v_n - v_m)\| \|u\| + \|v_n - v_m\| \|\nabla u\| \\ &\leq (\|T(v_n - v_m)\| + \|v_n - v_m\|) \|u\|_{H^1(\Omega)} \\ &\leq C_E (\|T(v_n - v_m)\| + \|v_n - v_m\|) \|f\|_{H^{1/2}(\partial\Omega)}. \end{aligned}$$

This in turn proves that the limit $\boldsymbol{\sigma} \cdot \mathbf{n} \gamma v$ of $\boldsymbol{\sigma} \cdot \mathbf{n} \gamma v_n$ exists in $H^{-1/2}(\partial\Omega)$. Since $\boldsymbol{\sigma} \cdot \mathbf{n}$ is a pointwise invertible matrix (in fact $(\boldsymbol{\sigma} \cdot \mathbf{n})^2 = 1$) with C^1 -entries, the same conclusion holds for γv .

Assume now that $v \in \mathcal{D}(D^*)$ and that $u \in \mathcal{D}(D)$, then $f := \gamma u = P_+ f$ and

$$i \int_{\partial\Omega} (\gamma v, \boldsymbol{\sigma} \cdot \mathbf{n} f)_{\mathbb{C}^2} = \int_{\Omega} (T v, u)_{\mathbb{C}^2} - (v, D u)_{\mathbb{C}^2} = \langle D^* v, u \rangle - \langle v, D u \rangle = 0.$$

This shows that $0 = P_+ \boldsymbol{\sigma} \cdot \mathbf{n} \gamma v$. A short calculation shows that $P_+ \boldsymbol{\sigma} \cdot \mathbf{n} = \boldsymbol{\sigma} \cdot \mathbf{n} P_-$ implying that $\boldsymbol{\sigma} \cdot \mathbf{n} P_- \gamma v = 0$ and the proof is finished. \square

The next lemma shows that improving the regularity of the traces is all that is left to do.

Lemma 2.4. *If $v \in \mathcal{K}$ and $\gamma v \in H^{1/2}(\partial\Omega, \mathbb{C}^2)$, then $v \in H^1(\Omega, \mathbb{C}^2)$.*

Proof. Let $v \in \mathcal{K}$ with $\gamma v \in H^{1/2}(\partial\Omega)$. By replacing v by $v - E(\gamma(v))$, where $E : H^{1/2}(\partial\Omega) \mapsto H^1(\Omega)$ is the (continuous) extension operator, it suffices to consider the case when $\gamma v = 0$.

Write $w := T v \in L^2(\Omega)$. Next we show that

$$(6) \quad \langle v, T \varphi \rangle = \langle w, \varphi \rangle, \quad \text{for all } \varphi \in C^\infty(\overline{\Omega}, \mathbb{C}^2).$$

Let $(v_n)_{n \in \mathbb{N}}$ be a $C^\infty(\overline{\Omega})$ -sequence approximating v in the \mathcal{K} -norm. Then by Lemma 2.3, $\gamma v_n \rightarrow \gamma v = 0$ in $H^{-1/2}(\partial\Omega)$. We calculate for $\varphi \in C^\infty(\overline{\Omega})$ using (1)

$$\begin{aligned} \langle v, T \varphi \rangle &= \lim_{n \rightarrow \infty} \langle v_n, T \varphi \rangle = \lim_{n \rightarrow \infty} \left(\langle T v_n, \varphi \rangle - i \int_{\partial\Omega} (\gamma v_n, \mathbf{n} \cdot \boldsymbol{\sigma} \gamma \varphi)_{\mathbb{C}^2} \right) \\ &= \langle w, \varphi \rangle, \end{aligned}$$

where the boundary term vanishes since $\gamma \varphi \in H^{1/2}(\partial\Omega)$. This proves (6).

Let \tilde{v} and \tilde{w} be the extensions by zero to $L^2(\mathbb{R}^2)$ of v and w , respectively. Then, by (6)

$$(7) \quad T \tilde{v} = \tilde{w}, \quad \text{in } \mathcal{D}'(\mathbb{R}^2).$$

From this we conclude that $\tilde{v} \in H^1(\mathbb{R}^2)$ and thus $v \in H^1(\Omega)$. This finishes the proof. \square

In order to take advantage of the special structure of the Dirac operator, it will be convenient to identify $\mathbf{x} \in \mathbb{R}^2$ with the complex number $z = x_1 + ix_2$. In this notation, the Dirac operator reads

$$Tu(z) = -2i \begin{pmatrix} 0 & \partial_z \\ \partial_{z^*} & 0 \end{pmatrix} u(z) = -2i \begin{pmatrix} \partial_z u_2(z) \\ \partial_{z^*} u_1(z) \end{pmatrix},$$

where we introduced the Cauchy-Riemann derivatives $\partial_z := \frac{1}{2}(\partial_1 - i\partial_2)$ and $\partial_{z^*} := \frac{1}{2}(\partial_1 + i\partial_2)$. In addition, we introduce the Cauchy kernel

$$(Kf)(\zeta) = \frac{1}{2\pi i} \int_{\partial\Omega} \frac{f(z)}{z - \zeta} dz$$

and its formal conjugate

$$(\overline{K}f)(\zeta) = \frac{-1}{2\pi i} \int_{\partial\Omega} \frac{f(z)}{z^* - \zeta^*} dz^*.$$

With these definitions we construct an operator on $C^\infty(\partial\Omega, \mathbb{C}^2)$ by setting

$$S = \begin{pmatrix} K & 0 \\ 0 & \overline{K} \end{pmatrix}.$$

Actually, $-2\gamma S \boldsymbol{\sigma} \cdot \mathbf{n}$ coincides with the Calderón projector for the Dirac operator as defined for instance in [7, Chapter 12].

2.2. The Cauchy kernel on the unit circle. On the unit circle \mathbb{S} the operators K and \overline{K} are explicit when acting on the standard basis. For this reason we will first establish all the necessary properties on the disc, $\Omega = \mathbb{D}$, and then translate them to general domains essentially by using the Riemann Mapping Theorem.

Define the orthonormal basis

$$e_n(\theta) = (2\pi)^{-1/2} e^{in\theta} \in L^2(\mathbb{S}^1),$$

in the standard parametrization of \mathbb{S}^1 . An explicit calculation yields,

$$(8) \quad Ke_n(\zeta) = \begin{cases} (2\pi)^{-1/2} \zeta^n, & n \geq 0, \\ 0, & n < 0, \end{cases}$$

and

$$\overline{K}e_n(\zeta) = \begin{cases} 0, & n > 0, \\ (2\pi)^{-1/2} (\zeta^*)^{|n|}, & n \leq 0. \end{cases}$$

Furthermore for L^2 -functions on the unit circle, we will denote the Fourier coefficients

$$\widehat{f}(n) = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} f(\theta) e^{-in\theta} d\theta = \langle e_n, f \rangle.$$

We set for $s \in \mathbb{R}$

$$\|f\|_{H^s}^2 = \sum_{n \in \mathbb{Z}} (|n| + 1)^{2s} |\widehat{f}(n)|^2,$$

where $\widehat{f}(n)$ is understood in the sense of distributions for $s < 0$.

The properties of K and \overline{K} that we will need are grouped in the following proposition.

Proposition 2.5. *If $\Omega = \mathbb{D}$ and K, \overline{K} are defined as above, then for all $s \in [-1/2, 1/2]$*

i) K and \overline{K} extend to bounded operators from $H^{-1/2}(\mathbb{S})$ to $L^2(\mathbb{D})$.

- ii) For all $f \in H^s(\mathbb{S})$ we have $\partial_{z^*} Kf = 0$ and $\partial_z \overline{K}f = 0$ with derivatives taken in the sense of distributions.
- iii) γK and $\gamma \overline{K}$ extend to bounded operators on $H^s(\mathbb{S})$ and they are self-adjoint projections onto $\text{span}\{e_n | n \geq 0\}$ and $\text{span}\{e_n | n \leq 0\}$, respectively.
- iv) $\gamma K + \gamma \overline{K} = 1 + \langle e_0, \cdot \rangle e_0$ when acting on $H^s(\mathbb{S})$.
- v) For $\beta \in C^1(\mathbb{S})$ and $s = -1/2$ or $s = 0$ the commutators $[\beta, \gamma K]$ and $[\beta, \gamma \overline{K}]$ are bounded from $H^s(\mathbb{S})$ to $H^{s+1/2}(\mathbb{S})$.

Proof. Point iv) is a direct consequence of iii). We will prove the remaining points for K only, since the same ideas apply to \overline{K} . Also, it is sufficient to establish these properties for continuous functions, since all statements extend to general elements of H^s by density.

In this setting, point i) follows from (8), since $\langle \zeta^n, \zeta^k \rangle = \frac{\pi}{n+1} \delta_{n,k}$ and

$$\|Kf\|_{L^2}^2 = \sum_{n,k \geq 0} \widehat{f}(n)^* \widehat{f}(k) \langle Ke_n, Ke_k \rangle = \sum_{n \geq 0} \frac{1}{2n+2} |\widehat{f}(n)|^2 \leq \|f\|_{H^{-1/2}}^2.$$

The proof of ii) is straightforward. Using (8) again we have that

$$(\gamma K)e_n = \begin{cases} e_n, & n \geq 0, \\ 0, & n < 0, \end{cases}$$

which establishes point iii).

To see v), we take $s = -1/2$ or $s = 0$, fix $f \in C^1(\partial\Omega)$ and compute the Fourier coefficients of $[\beta, \gamma K]f = \beta \gamma Kf - \gamma K(\beta f)$,

$$\sqrt{2\pi}([\beta, \gamma K]f)^\wedge(n) = \begin{cases} \sum_{k \geq 0} \widehat{\beta}(n-k) \widehat{f}(k) - \sum_{k \in \mathbb{Z}} \widehat{\beta}(n-k) \widehat{f}(k), & n \geq 0, \\ \sum_{k \geq 0} \widehat{\beta}(n-k) \widehat{f}(k), & n < 0. \end{cases}$$

By Cauchy-Schwarz,

$$\begin{aligned} 2\pi |([\beta, \gamma K]f)^\wedge(n)|^2 &\leq \begin{cases} \sum_{k < 0} |\widehat{\beta}(n-k)|^2 (|k|+1)^{-2s} \sum_{k < 0} |\widehat{f}(k)|^2 (|k|+1)^{2s}, & n \geq 0, \\ \sum_{k \geq 0} |\widehat{\beta}(n-k)|^2 (|k|+1)^{-2s} \sum_{k \geq 0} |\widehat{f}(k)|^2 (|k|+1)^{2s}, & n < 0, \end{cases} \\ &\leq \|f\|_{H^s}^2 \begin{cases} \sum_{k < 0} |\widehat{\beta}(n-k)|^2 (|k|+1)^{-2s}, & n \geq 0, \\ \sum_{k \geq 0} |\widehat{\beta}(n-k)|^2 (|k|+1)^{-2s}, & n < 0. \end{cases} \end{aligned}$$

Therefore, we obtain

$$\begin{aligned} \|[\beta, \gamma K]f\|_{H^{s+1/2}}^2 &= \sum_{n \in \mathbb{Z}} (|n|+1)^{2s+1} |([\beta, \gamma K]f)^\wedge(n)|^2 \\ &\leq \|f\|_{H^s}^2 \left(\sum_{\substack{n \geq 0 \\ k < 0}} (|n|+1)^{2s+1} (|k|+1)^{-2s} |\widehat{\beta}(n-k)|^2 \right. \\ &\quad \left. + \sum_{\substack{n < 0 \\ k \geq 0}} (|n|+1)^{2s+1} (|k|+1)^{-2s} |\widehat{\beta}(n-k)|^2 \right). \end{aligned}$$

Since either $2s+1 = 0$ or $s = 0$ we get

$$(|n|+1)^{2s+1} (|k|+1)^{-2s} \leq |n|+|k|+1 = |n-k|+1,$$

where the last equality holds since n and k have opposite signs in the sums we are considering. This allows us to conclude that

$$\begin{aligned} \|[\beta, \gamma K]f\|_{H^{s+1/2}}^2 &\leq \|f\|_{H^s}^2 \left(\sum_{\substack{n \geq 0 \\ k < 0}} (|n-k|+1) |\widehat{\beta}(n-k)|^2 \right. \\ &\quad \left. + \sum_{\substack{n < 0 \\ k \geq 0}} (|n-k|+1) |\widehat{\beta}(n-k)|^2 \right) \\ &\leq \|f\|_{H^s}^2 \left(\sum_{m \geq 1} (|m|+1)^2 |\widehat{\beta}(m)|^2 + \sum_{m \leq -1} (|m|+1)^2 |\widehat{\beta}(m)|^2 \right) \\ &\leq \|f\|_{H^s}^2 \|\beta\|_{H^1}^2, \end{aligned}$$

which finishes the proof. \square

The following lemma relates the operators K , \overline{K} and S to our problem at hand.

Lemma 2.6. *Let $\Omega = \mathbb{D}$ and assume $v \in \mathcal{K}$. Then $\gamma S(\boldsymbol{\sigma} \cdot \mathbf{n} \gamma v) \in H^{1/2}(\mathbb{S}, \mathbb{C}^2)$.*

Proof. Take a test function $f \in C^\infty(\mathbb{S}, \mathbb{C}^2)$ and a sequence $(v_n)_{n \in \mathbb{N}} \subset C^1(\overline{\mathbb{D}}, \mathbb{C}^2)$ approaching v in \mathcal{K} . By Proposition 2.5 *iii*), γS is self-adjoint, thus using (1)

$$\begin{aligned} \int_{\mathbb{S}} (\gamma S(\boldsymbol{\sigma} \cdot \mathbf{n} \gamma v_n), f)_{\mathbb{C}^2} &= \int_{\mathbb{S}} (\gamma v_n, \boldsymbol{\sigma} \cdot \mathbf{n} \gamma S f)_{\mathbb{C}^2} \\ &= -i \langle T v_n, S f \rangle + i \langle v_n, T S f \rangle. \end{aligned}$$

The last term above cancels since, by Proposition 2.5 *ii*), $T S f = 0$. Thus, in view of Proposition 2.5 *i*)

$$\left| \int_{\mathbb{S}} (\gamma S(\boldsymbol{\sigma} \cdot \mathbf{n} \gamma v_n), f)_{\mathbb{C}^2} \right| \leq \|T v_n\|_{L^2(\mathbb{D})} \|S f\|_{L^2(\mathbb{D})} \leq C_K \|T v_n\|_{L^2(\mathbb{D})} \|f\|_{H^{-1/2}(\mathbb{S})}.$$

Taking the limit as $n \rightarrow \infty$ on both sides we see that $\gamma S(\boldsymbol{\sigma} \cdot \mathbf{n} \gamma v)$ extends to a continuous functional on $H^{-1/2}$, and thus can be identified with a function in $H^{1/2}$. \square

The next lemma allows us to conclude the proof of self-adjointness when $\Omega = \mathbb{D}$, see Remark 5.

Lemma 2.7. *Let $\Omega = \mathbb{D}$ and β be a nowhere vanishing $C^1(\mathbb{S})$ -function. Assume that $v \equiv \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \in \mathcal{K}$ and that $\gamma v_1 = \beta \gamma v_2$ as an equality in $H^{-1/2}(\mathbb{S})$. Then $\gamma v \in H^{1/2}(\mathbb{S}, \mathbb{C}^2)$.*

Remark 5. In view of Lemma 2.3, $v \in \mathcal{D}(D^*)$ satisfies the hypotheses of Lemma 2.7 with $\beta = \frac{t^* \cos \eta}{1 - \sin \eta}$. Thus, according to Lemma 2.4, $v \in H^1(\mathbb{D}, \mathbb{C}^2)$ satisfies the boundary conditions. In particular, $\mathcal{D}(D^*) \subset \mathcal{D}(D)$.

Proof. Let us write

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \begin{pmatrix} 0 & n^* \\ n & 0 \end{pmatrix}.$$

In order to apply Lemma 2.6, we define the spinor $f = \boldsymbol{\sigma} \cdot \mathbf{n} \gamma v$. Due to the boundary condition we have that $f_2 = \tilde{\beta} f_1$ where $\tilde{\beta} = (n)^2 \beta$ is a C^1 -function. In this notation Lemma 2.6 states that

$$(9) \quad \gamma K f_1 \in H^{1/2}, \quad \gamma \overline{K} f_2 \in H^{1/2}.$$

Now we write

$$(10) \quad \gamma K f_2 = \gamma K(\tilde{\beta} f_1) = \tilde{\beta} \gamma K f_1 - [\tilde{\beta}, \gamma K] f_1.$$

Clearly $\tilde{\beta} \gamma K f_1$ is in $H^{1/2}$. By Proposition 2.5 *v*), the term with the commutator is in L^2 , so $\gamma K f_2 \in L^2$ as well. This together with (9) gives that $f_2 \in L^2$, in view of Proposition 2.5 *iv*). Since $\tilde{\beta}$ does not vanish, f_1 is also in L^2 due to the boundary conditions. With this improved regularity we return to (10) and observe that, due to Proposition 2.5 *v*), $[\tilde{\beta}, \gamma K] f_1$ is in $H^{1/2}$ so the same holds for $\gamma K f_2$. Again using the complementarity of the projections and the fact $\tilde{\beta}$ does not vanish, we conclude $f_1, f_2 \in H^{1/2}$. \square

2.3. Riemann mapping and the proof of Theorem 1.1. We first give the proof in the case where Ω is simply connected. The case of multiply connected domains will be commented on at the end. Since $\partial\Omega$ is C^2 , there exists a C^1 conformal mapping (up to the boundary) $F : \overline{\Omega} \rightarrow \overline{\mathbb{D}}$ with inverse G [14, Theorem 3.5, p. 48]. Consider the map U defined by $(Uf)(z) := f(G(z))$ mapping functions on $\overline{\Omega}$ to functions on $\overline{\mathbb{D}}$. By restriction (and abuse of notation), U also maps functions on $\partial\Omega$ to functions on \mathbb{S} .

Lemma 2.8. *When Ω is simply connected and has C^2 -boundary, the map U defines a bounded bijection from $L^2(\Omega)$ to $L^2(\mathbb{D})$ with bounded inverse. Furthermore, $U : H^s(\Omega) \rightarrow H^s(\mathbb{D})$ is bounded with bounded inverse, for all $s \in [-1, 1]$.*

Similarly, $U : H^s(\partial\Omega) \rightarrow H^s(\mathbb{S})$ is bounded with bounded inverse, for all $s \in [-1, 1]$.

Finally, if $v \in \mathcal{D}(D^)$, then $Uv = (u_1, u_2) \in \mathcal{K}(\mathbb{D})$ and on the boundary $\gamma u_1 = \beta \gamma u_2$ as an identity in $H^{-1/2}(\mathbb{S})$, where $\beta = U(\frac{t^* \cos(\eta)}{1 - \sin(\eta)})$ is $C^1(\mathbb{S})$.*

Proof. Since F, G have bounded derivatives on $\overline{\Omega}$ (resp $\overline{\mathbb{D}}$) the map $L^2(\Omega) \ni v \mapsto u := Uv = v \circ G \in L^2(\Omega)$ is a bounded bijection with bounded inverse. By direct differentiation one verifies that U is also bounded from $H^1(\Omega)$ to $H^1(\mathbb{D})$ with bounded inverse. By interpolation and duality one finds that also $U : H^s(\Omega) \rightarrow H^s(\mathbb{D})$ is bounded with bounded inverse, for all $s \in [-1, 1]$.

The same argument as in the interior applies on the boundary, so we see that $U : H^s(\partial\Omega) \rightarrow H^s(\mathbb{S})$ is bounded with bounded inverse, for all $s \in [-1, 1]$.

Suppose now that $v = (v_1, v_2) \in \mathcal{D}(D^*)$. Then, since $\partial_{z^*} G = 0$, we have by the chain rule,

$$\partial_z u_2 = G' \partial_z v_2 \in L^2(\mathbb{D}), \quad \partial_{z^*} u_1 = (G')^* \partial_{z^*} v_1 \in L^2(\mathbb{D}).$$

Finally, the boundary condition $\gamma u_1 = \beta \gamma u_2$ follows from the boundary condition satisfied by v , see Lemma 2.3. \square

Now we can conclude the proof of the self-adjointness of D .

Proof of Theorem 1.1. Simply connected case. Fix $v \in \mathcal{D}(D^*)$. By Lemmas 2.3 and 2.4, we only have to prove that v has a well-defined trace in $H^{1/2}(\partial\Omega)$. By Lemma 2.8, this is equivalent to showing that $\gamma u := \gamma Uv \in H^{1/2}(\mathbb{S})$, where U is the map defined above. By the same lemma, $u \in \mathcal{K}$ and its components u_1, u_2 satisfy the boundary condition $\gamma u_1 = \beta \gamma u_2$, with $\beta = U(\frac{t^* \cos(\eta)}{1 - \sin(\eta)})$. Since β vanishes nowhere by assumption, we can apply Lemma 2.7 and conclude the proof of the theorem in this case.

Multiply connected case. It clearly suffices to consider connected Ω . Suppose that $\partial\Omega$ is made up of the simple, regular curves $\Gamma_0, \dots, \Gamma_n$, with $n \geq 1$. Let Ω_j be the interior components of $\mathbb{R}^2 \setminus \Gamma_j$ (given by the Jordan Curve Theorem). Let Γ_0 be the exterior boundary. Since Ω is connected, $\Omega \subset \Omega_0$ and $\Omega \subset \mathbb{R}^2 \setminus \overline{\Omega_j}$ for $j \geq 1$.

Let first $F_0 : \Omega_0 \rightarrow \mathbb{D}$ be the conformal (Riemann) map and let $U_0 : L^2(\Omega) \rightarrow L^2(U_0(\Omega))$ be the push-forward map as in Lemma 2.8. Proceeding as in the proof in the simply connected case, using U_0 instead of U , one concludes the desired $H^{1/2}$ -regularity on the boundary component Γ_0 .

For $j \in \{1, \dots, n\}$ let $z_j \in \Omega_j$. To obtain the $H^{1/2}$ -regularity on the boundary component Γ_j , one first applies the fractional transformation $I_j(z) = (z - z_j)^{-1}$. After this transformation, $I_j(\Gamma_j)$ is the external boundary of $I_j(\Omega)$ and one can proceed as in the previous case. Notice that since $z_j \in \Omega_j$, the map I_j (and its inverse) has bounded derivatives to all orders in Ω and therefore preserves Sobolev spaces in a similar manner to Lemma 2.8. This finishes the proof of Theorem 1.1. \square

3. LOWER BOUND FOR SIMPLY CONNECTED DOMAINS

The goal of this section is to prove Theorem 1.2, which gives a lower bound on the size of the spectral gap of a graphene sample around zero, for some of the physically relevant boundary conditions. In [4] the following lower bound for the eigenvalues of the (classical) Dirac operator on *closed* surfaces M of genus one (surfaces homeomorphic to a sphere) is proved:

$$(11) \quad \lambda^2 \geq \frac{4\pi}{\text{area}(M)}.$$

The bound we obtain for an open and simply connected surface Ω with infinite mass boundary conditions ($\eta = 0$ or $\eta = \pi$) is

$$\lambda^2 \geq \frac{2\pi}{|\Omega|}.$$

Before going into the proof, let us give a heuristic interpretation of this result. At least formally, these particular boundary conditions provide the possibility to extend spinors in $\mathcal{D}(D)$ to the *invertible double* $\tilde{\Omega}$, which is the closed surface obtained by glueing Ω to its mirror image. Details of this construction can be found in [7, chapter 9]. The bottomline is that an eigenspinor u of D can be extended to an eigenspinor \tilde{u} of the extended Dirac operator \tilde{D} by identifying $\tilde{u} \approx (u, -u)$. Then, the bound of Theorem 1.2 follows from Bär's bound (11), since $\text{area}(\tilde{\Omega}) = 2|\Omega|$.

This argument can be made rigorous by considering closed surfaces $\tilde{\Omega}_\epsilon \subset \mathbb{R}^3$ consisting of two copies of Ω in parallel planes with a distance ϵ between them, joined smoothly by a *ribbon* of width proportional to ϵ . There is some work involved in computing explicitly the extension of D to the curved ribbon and in checking that eigenspinors can be extended correspondingly. One has to make sure that the contribution of the curved part to the Rayleigh quotient tends to zero with ϵ in order to obtain the result.

If Ω is not simply connected, we can still perform the doubling construction, but the resulting closed manifold will be homeomorphic to a torus or a surface of higher genus. In principle, this case can be treated using the results in [3] that extend (11).

Instead of going through calculations with spinors on curved surfaces we will use the strategy from [4] taking care of the boundary terms. The boundary conditions for constant $\eta \notin \{0, \pi\}$ do not have the above described *doubling property*. However, one can extend the result for $\eta = 0$ to the general case, as the following lemma shows.

Lemma 3.1. *Take D_η satisfying the hypotheses of Theorem 1.2, and*

$$B = \min(|\cos \eta / (1 - \sin \eta)|, |(1 - \sin \eta) / \cos \eta|).$$

If λ_η is the eigenvalue of D_η of smallest absolute value, then

$$\lambda_\eta^2 \geq B^2 \lambda_0^2.$$

Proof. Assume $\eta \in (0, \pi/2)$ such that $B = (1 - \sin \eta) / \cos \eta \in (0, 1)$. Take an eigenspinor u of D_η associated to the eigenvalue λ_η . Writing out the boundary conditions explicitly, we obtain $u_2 = Btu_1$ on $\partial\Omega$. Then, we may write $u = u_0 + u_z$, where $u_0 = \begin{pmatrix} B & 0 \\ 0 & 1 \end{pmatrix} u$. This gives $u_0 \in \mathcal{D}(D_0)$, while $u_z \in \mathcal{D}(D_{\pi/2})$. Now we have

$$\lambda_\eta^2 \|u\|^2 = \|Tu_0 + Tu_z\|^2 = \|Tu_0\|^2 + \|Tu_z\|^2 + 2 \operatorname{Re} \langle Tu_0, Tu_z \rangle.$$

The last two terms can be combined using the fact that u_z has only its first component nonzero. We get

$$\begin{aligned} \|Tu_z\|^2 + 2 \operatorname{Re} \langle Tu_0, Tu_z \rangle &= (1 - B)^2 \|2\partial_{z^*} u_1\|^2 + 2B(1 - B) \|2\partial_{z^*} u_1\|^2 \\ &= (1 - B^2) \|2\partial_{z^*} u_1\|^2. \end{aligned}$$

Since $|B| \leq 1$ by definition, we have

$$\lambda_\eta^2 \|u\|^2 \geq \|D_0 u_0\|^2 \geq \lambda_0^2 \|u_0\|^2 \geq \lambda_0^2 B^2 \|u\|^2,$$

which is the desired inequality. The other cases are analogous: it suffices to define $u_0 = \begin{pmatrix} B & 0 \\ 0 & -1 \end{pmatrix} u$ when η lies in $(\pi/2, \pi)$ or $u_0 = \begin{pmatrix} \pm 1 & 0 \\ 0 & B \end{pmatrix} u$ for $\eta \in (\pi, 3\pi/2)$ and $\eta \in (3\pi/2, 2\pi)$. \square

Proof of Theorem 1.2. By the previous lemma we can restrict our attention to $\eta = 0$, so to simplify notations, we will write $D_0 = D$. We start by a calculation for C^1 -spinors $u, v \in \mathcal{D}(D)$

$$\begin{aligned} (Du, Dv) &= \sum_{k,j} \int_{\Omega} (\partial_k u, \sigma_k \sigma_j \partial_j v)_{\mathbb{C}^2} \\ &= \sum_k \int_{\Omega} (\partial_k u, \partial_k v)_{\mathbb{C}^2} + i \sum_{k,j} \epsilon_{kj} \int_{\Omega} (\partial_k u, \sigma_3 \partial_j v)_{\mathbb{C}^2}. \end{aligned}$$

In the second term we can integrate by parts using the antisymmetry of ϵ_{kj} and introduce the tangent vector at the boundary $\mathbf{t} = (-\mathbf{n}_2, \mathbf{n}_1)$. We obtain

$$\begin{aligned} \sum_{k,j} i \epsilon_{kj} \int_{\Omega} (\partial_k u, \sigma_3 \partial_j v)_{\mathbb{C}^2} &= \sum_{k,j} i \epsilon_{kj} \int_{\Omega} \partial_k (u, \sigma_3 \partial_j v)_{\mathbb{C}^2} \\ &= \sum_{k,j} i \epsilon_{kj} \int_{\partial\Omega} \mathbf{n}_k (u, \sigma_3 \partial_j v)_{\mathbb{C}^2} \\ &= i \int_{\partial\Omega} (u, \sigma_3 \mathbf{t} \cdot \nabla v)_{\mathbb{C}^2}. \end{aligned}$$

Since only the tangent derivative is involved, this term depends solely on the boundary values of u and v . We can explicitly write out the spinor components and introduce the boundary condition in the form $u_2 = tu_1$:

$$(u, \sigma_3 \mathbf{t} \cdot \nabla v)_{\mathbb{C}^2} = u_1^* \mathbf{t} \cdot \nabla v_1 - u_2^* \mathbf{t} \cdot \nabla v_2 = -u_1^* v_1 t^* t' = -iu_1^* v_1 \kappa(s)$$

In the last equality, we used $\partial_s \mathbf{t}(s) = -\kappa(s) \mathbf{n}(s)$ (see Subsection 1.2). By density,

$$(12) \quad (Du, Dv) = (\nabla u, \nabla v) + \frac{1}{2} \int_{\partial\Omega} (u, v)_{\mathbb{C}^2} (s) \kappa(s) ds$$

holds for all $u, v \in \mathcal{D}(D)$.

For a real constant α and a real C^1 -function f we define a modified connection

$$\tilde{\partial}_j = \partial_j - i\alpha\sigma_j - \sigma_f\sigma_j,$$

where $\sigma_f := \boldsymbol{\sigma} \cdot \nabla f$. For spinor fields u, v we compute the product

$$\begin{aligned} \sum_j \left(\tilde{\partial}_j u, \tilde{\partial}_j v \right)_{\mathbb{C}^2} &= \sum_j \left((\partial_j u, \partial_j v)_{\mathbb{C}^2} + \alpha^2 (\sigma_j u, \sigma_j v)_{\mathbb{C}^2} + (\sigma_f \sigma_j u, \sigma_f \sigma_j v)_{\mathbb{C}^2} \right. \\ &\quad \left. - (\partial_j u, (i\alpha\sigma_j + \sigma_f \sigma_j) v)_{\mathbb{C}^2} - ((i\alpha\sigma_j + \sigma_f \sigma_j) u, \partial_j v)_{\mathbb{C}^2} \right. \\ &\quad \left. + i\alpha (\sigma_j u, \sigma_f \sigma_j v)_{\mathbb{C}^2} - i\alpha (\sigma_f \sigma_j u, \sigma_j v)_{\mathbb{C}^2} \right) \\ &= (\nabla u, \nabla v)_{\mathbb{C}^2} + (2\alpha^2 + 2|\nabla f|^2) (u, v)_{\mathbb{C}^2} \\ &\quad - \alpha ((Du, v)_{\mathbb{C}^2} + (u, Dv)_{\mathbb{C}^2}) \\ &\quad - \sum_j ((\partial_j u, \sigma_f \sigma_j v)_{\mathbb{C}^2} + (\sigma_f \sigma_j u, \partial_j v)_{\mathbb{C}^2}). \end{aligned}$$

We are interested in the integral over Ω of the above quantity with the weight e^{-2f} . If $u, v \in \mathcal{D}(D^2)$, then we obtain using (12)

$$\begin{aligned} \langle e^{-2f} u, D^2 v \rangle &= \langle D e^{-2f} u, D v \rangle \\ &= \langle \nabla e^{-2f} u, \nabla v \rangle + \int_{\partial\Omega} e^{-2f} \frac{\kappa}{2} (u, v)_{\mathbb{C}^2} \\ &= \int_{\Omega} e^{-2f} \left((\nabla u, \nabla v)_{\mathbb{C}^2} - 2 \sum_j (\partial_j f) (u, \partial_j v)_{\mathbb{C}^2} \right) + \int_{\partial\Omega} e^{-2f} \frac{\kappa}{2} (u, v)_{\mathbb{C}^2}. \end{aligned}$$

By the anticommutation relations, we obtain

$$\sum_j (\sigma_f \sigma_j u, \partial_j v)_{\mathbb{C}^2} = -i (u, \sigma_f D v)_{\mathbb{C}^2} + 2 \sum_j (\partial_j f) (u, \partial_j v)_{\mathbb{C}^2}$$

and by integration by parts

$$\begin{aligned} \sum_j \int_{\Omega} e^{-2f} (\partial_j u, \sigma_f \sigma_j v)_{\mathbb{C}^2} &= -i \langle e^{-2f} u, \sigma_f D v \rangle + \langle (-\Delta f + 2|\nabla f|^2) e^{-2f} u, v \rangle \\ &\quad + \int_{\partial\Omega} e^{-2f} (u, \sigma_f \boldsymbol{\sigma} \cdot \mathbf{n} v)_{\mathbb{C}^2}. \end{aligned}$$

Inserting these identities, we obtain

$$\begin{aligned}
\sum_j \int_{\Omega} e^{-2f} \left(\tilde{\partial}_j u, \tilde{\partial}_j v \right)_{\mathbb{C}^2} &= \langle e^{-2f} u, D^2 v \rangle + 2 \sum_j \langle e^{-2f} u, (\partial_j f) \partial_j v \rangle \\
&+ \langle e^{-2f} (2\alpha^2 + 2|\nabla f|^2) u, v \rangle - \alpha \langle e^{-2f} u, Dv \rangle - \alpha \langle e^{-2f} Du, v \rangle \\
&+ 2i \langle e^{-2f} u, \sigma_f Dv \rangle + \langle e^{-2f} u, \Delta f v \rangle \\
&- 2 \sum_j \langle e^{-2f} u, (\partial_j f) \partial_j v \rangle - 2 \langle e^{-2f} |\nabla f|^2 u, v \rangle \\
&+ \int_{\partial\Omega} e^{-2f} \left(-\frac{\kappa}{2} (u, v)_{\mathbb{C}^2} - (u, \sigma_f \boldsymbol{\sigma} \cdot \mathbf{n} v)_{\mathbb{C}^2} \right).
\end{aligned}$$

Note that the four terms containing first derivatives of f cancel exactly. Applying this identity with $v = u$ and $Du = \lambda u$, this reduces to

$$\begin{aligned}
\sum_j \int_{\Omega} e^{-2f} \left(\tilde{\partial}_j u, \tilde{\partial}_j u \right)_{\mathbb{C}^2} &= (\lambda^2 + 2\alpha^2 - 2\alpha\lambda) \|e^{-f} u\|^2 \\
&+ 2i\lambda \langle u, \sigma_f u \rangle + \langle e^{-2f} u, \Delta f u \rangle \\
&+ \int_{\partial\Omega} e^{-2f} \left(-\frac{\kappa}{2} (u, u)_{\mathbb{C}^2} - (u, \sigma_f \boldsymbol{\sigma} \cdot \mathbf{n} u)_{\mathbb{C}^2} \right).
\end{aligned}$$

Now we use the fact that the left hand side is real and nonnegative, and choose $\alpha = \lambda/2$ in order to minimize the coefficient of the first term. We obtain the inequality

$$0 \leq \frac{\lambda^2}{2} \|e^{-f} u\|^2 + \langle e^{-2f} u, (\Delta f) u \rangle + \int_{\partial\Omega} e^{-2f} \left(-\frac{\kappa}{2} (u, u)_{\mathbb{C}^2} - \operatorname{Re} (u, \sigma_f \boldsymbol{\sigma} \cdot \mathbf{n} u)_{\mathbb{C}^2} \right).$$

Using anticommutation relations, $\operatorname{Re} (u, \sigma_f \boldsymbol{\sigma} \cdot \mathbf{n} u)_{\mathbb{C}^2} = (\mathbf{n} \cdot \nabla f) (u, u)_{\mathbb{C}^2}$, so we obtain

$$\frac{\lambda^2}{2} \|e^{-f} u\|^2 \geq - \langle e^{-2f} u, (\Delta f) u \rangle + \int_{\partial\Omega} e^{-2f} (u, u)_{\mathbb{C}^2} \left(\frac{\kappa}{2} + \mathbf{n} \cdot \nabla f \right).$$

This suggests to take f solving, for some $C \in \mathbb{R}$,

$$(13) \quad \begin{cases} \Delta f = C & \text{in } \Omega, \\ \mathbf{n} \cdot \nabla f = -\kappa/2 & \text{in } \partial\Omega. \end{cases}$$

To see that such an f exists, set $f_0(x) = C|x|^2/4$. By [10, Theorem 3.40, p138], we can find f_h satisfying

$$\begin{cases} \Delta f_h = 0, & \text{in } \Omega, \\ \mathbf{n} \cdot \nabla f_h = -\kappa/2 - \mathbf{n} \cdot \nabla f_0, & \text{in } \partial\Omega, \end{cases}$$

provided $\int_{\partial\Omega} (-\kappa/2 - \mathbf{n} \cdot \nabla f_0) = 0$. But $\int_{\partial\Omega} \kappa = 2\pi$ and $\int_{\partial\Omega} \mathbf{n} \cdot \nabla f_0 = \int_{\Omega} \Delta f_0 = C|\Omega|$. So with the choice $C = -\pi/|\Omega|$, $f_h + f_0$ satisfies (13). The final result is

$$\lambda^2 \geq -2C = \frac{2\pi}{|\Omega|}.$$

□

Acknowledgments. This work has been supported by the Iniciativa Científica Milenio (Chile) through the Millenium Nucleus RC-120002 “Física Matemática”. R.B. has been supported by Fondecyt (Chile) Projects # 112-0836 and #114-1155.

S.F. acknowledges partial support from a Sapere Aude grant from the Danish Councils for Independent Research, Grant number DFF-4181-00221. E.S has been partially funded by Fondecyt (Chile) project # 114-1008. H. VDB. acknowledges support from Conicyt (Chile) through CONICYT-PCHA/Doctorado Nacional/2014. This work was carried out while S.F. was invited professor at Pontificia Universidad Católica de Chile. H.VDB. would like to thank Martin Chuaqui for interesting discussions.

APPENDIX A. APPLICATION TO THE TWO-VALLEY DESCRIPTION OF GRAPHENE

We would like to mention briefly some applications of our results to the full description of electronic excitations in graphene as a four-component spinor. In a convenient representation, the Hamiltonian becomes

$$H = \begin{pmatrix} T & 0 \\ 0 & T \end{pmatrix}.$$

In order to have a symmetric operator, the four-spinors should fullfil

$$P_-(A)\psi := \frac{1}{2}(1 - A)\psi = 0$$

at the boundary. Here A is a unitary matrix belonging to a four-parameter family (see [2] for its explicit form). For simplicity we will restrict our attention to the boundary conditions most commonly used in the physics literature:

A.1. Zigzag boundary conditions. In this case,

$$A = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix}$$

These boundary conditions do not mix the two valleys. We obtain two copies of $D_{\pi/2}$, which is not self-adjoint on $H^1(\Omega, \mathbb{C}^2)$ [17] and has zero as an eigenvalue of infinite multiplicity.

A.2. Infinite Mass boundary conditions. The matrix giving the boundary conditions here is

$$A = \begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{t} & 0 \\ 0 & -\boldsymbol{\sigma} \cdot \mathbf{t} \end{pmatrix}.$$

This does not mix the valleys either and gives a block diagonal operator with D_0 and D_π on the diagonal. This operator is self-adjoint with domain $\mathcal{D}(D_0) \oplus \mathcal{D}(D_\pi) \subset H^1(\Omega, \mathbb{C}^4)$ and the estimate of Theorem 1.2 holds.

A.3. Armchair boundary conditions. In this case,

$$A = \begin{pmatrix} 0 & \nu^* \boldsymbol{\sigma} \cdot \mathbf{t} \\ \nu \boldsymbol{\sigma} \cdot \mathbf{t} & 0 \end{pmatrix}$$

where $|\nu| = 1$. Using the unitary transformation

$$U_\nu = \begin{pmatrix} \nu 1_{\mathbb{C}^2} & 0 \\ 0 & 1_{\mathbb{C}^2} \end{pmatrix}$$

we can restrict our attention to the case $\nu = 1$. Consider the unitary transformation

$$U_p = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

corresponding to a permutation of the second and fourth spinor components. This transforms the boundary conditions in

$$\tilde{A} = U_p A U_p^* = \begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{t} & 0 \\ 0 & \boldsymbol{\sigma} \cdot \mathbf{t} \end{pmatrix},$$

and the Hamiltonian as

$$\tilde{H} = U_p H U_p^* = \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}.$$

After this transformation, a four-spinor ψ in the domain of \tilde{H} can be written as $\psi = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ with $u_1, u_2 \in \mathcal{D}(D_0)$. A short calculation shows that the same holds for the adjoints: $\phi \in \mathcal{D}(\tilde{H}^*)$ if and only if $\phi = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ with $v_1, v_2 \in \mathcal{D}(D_0^*)$. Thus, by Theorem 1.1, H is self-adjoint on $\mathcal{D}(H) \subset H^1(\Omega, \mathbb{C}^4)$. Furthermore,

$$\|\tilde{H}\psi\|^2 = \left\| \begin{pmatrix} D_0 u_2 \\ D_0 u_1 \end{pmatrix} \right\|^2 \geq \frac{2\pi}{|\Omega|} \|\psi\|^2.$$

In other words, the estimate of Theorem 1.2 holds in this case as well.

APPENDIX B. CONSTRUCTION OF A WEYL SEQUENCE

Here, we will construct a singular Weyl sequence to prove that, if $\cos \eta$ vanishes to second order at a point of $\partial\Omega$, then $0 \in \sigma_{\text{ess}}(D_\eta)$. In particular, this implies that if the boundary conditions on a part of the boundary are of zigzag-type, there are states, localized near this part of the boundary, with energy arbitrarily close to zero. This also shows that there is no self-adjoint realization of the corresponding operator on a domain included in $H^1(\Omega, \mathbb{C}^2)$.

We will assume for definiteness that η tends quadratically to $\frac{\pi}{2}$ at a point of the boundary. Then, the boundary conditions can be written $\gamma u_2 = B t \gamma u_1$, where $B = (1 - \sin \eta) / \cos \eta$. Our assumption implies then that $|B(s)| \leq C(s - s_0)^2$ and that $|\mathbf{t} \cdot \nabla B(s)| \leq C|s - s_0|$ for some $s_0 \in \partial\Omega$. We identify \mathbb{R}^2 with \mathbb{C} and assume for definiteness that $s_0 = 0$ and that $t(0) = i$. Then, we can find $R_0 > 0$ such that

$$(14) \quad \Omega \cap \{r e^{i\phi} | 0 \leq r \leq R_0, |\phi| \leq \pi/4\} = \emptyset.$$

Taking a smaller R_0 if necessary, we may also assume that B and t can be extended to C^1 -functions on $\overline{\Omega} \cap B(0, R_0)$, such that

$$\frac{|B(z)|}{|z|} + |\nabla B(z)| \leq C_B |z|, \quad |t| + |\nabla t| \leq C_t, \quad \text{for all } z \in \overline{\Omega} \cap B(0, R_0),$$

where C_B and C_t are positive constants. This is always possible since such constants exist for $z \in \partial\Omega$ and Ω has a C^2 -boundary. We also fix a cutoff function $\chi \in C^\infty(\mathbb{R}, [0, 1])$ such that $\chi(x) = 1$ for $x \leq 1/2$, $\chi(x) = 0$ for $x \geq 1$ and $|\chi'| \leq 3$. For $R \geq 0$, define $\chi_R(z) = \chi(|z|/R)$.

Now for $n \geq 1$, we set

$$u_n(z) = (z - s_n)^{-n} \begin{pmatrix} 1 \\ Bt \end{pmatrix}$$

for some $s_n > 0$. Notice that $v_n := \chi_{R_n} u_n \in \mathcal{D}(D_\eta)$ for some $R_n \leq R_0$. We have that

$$\|v_n\| \geq \|\chi_{R_n} (z - s_n)^{-n}\|.$$

On the other hand,

$$\begin{aligned} \|Tv_n\| &\leq \|\nabla \chi_{R_n} u_n\| + 2\|\chi_{R_n} \begin{pmatrix} \partial_z B t(z - s_n)^{-n} \\ \partial_{z^*} (z - s_n)^{-n} \end{pmatrix}\| \\ &\leq \frac{3}{R_n} \|\mathbf{1}_{[R_n/2, R_n]}(|z|)u_n\| + 2C_B C_t R_n \|\chi_{R_n} (z - s_n)^{-n}\| \\ &\quad + nC_t \|\chi_{R_n} B(z - s_n)^{-n-1}\|, \end{aligned}$$

where $\mathbf{1}_I$ is the indicator function on an interval $I \subset \mathbb{R}$. The last term can be estimated further by observing that, within $\text{supp } \chi_{R_n} \cap \Omega$,

$$\frac{|B|}{|z - s_n|} \leq C_B \frac{|z|^2}{|z - s_n|} \leq C_B R_n \sqrt{2},$$

where the last inequality holds in view of (14). Thus, we obtain

$$\frac{\|Tv_n\|}{\|v_n\|} \leq \frac{3}{R_n} \frac{\|\mathbf{1}_{[R_n/2, R_n]}(|z|)u_n\|}{\|\chi_{R_n} (z - s_n)^{-n}\|} + C_B C_t (2 + \sqrt{2}n) R_n.$$

We now fix $R_n \leq R_0$ such that the second term in the above equation is smaller than $1/2n$. In the first term, we note that, as $s_n \searrow 0$ for a fixed R_n , the numerator stays bounded while the denominator increases to $+\infty$. Thus, by choosing a sufficiently small s_n , we obtain

$$\frac{\|Tv_n\|}{\|v_n\|} \leq \frac{1}{n}.$$

In addition, the sequence $v_n/\|v_n\|$ converges weakly to zero, so it is a singular Weyl sequence, which proves $0 \in \sigma_{\text{ess}}(D_\eta)$.

REFERENCES

- [1] R. A. Adams, *Sobolev spaces*, Academic Press, New York-London, 1975, Pure and Applied Mathematics, Vol. 65.
- [2] A. R. Akhmerov and C. W. J. Beenakker, *Boundary conditions for Dirac fermions on a terminated honeycomb lattice*, Phys. Rev. B **77** (2008), 085423.
- [3] B. Ammann and C. Bär, *Dirac eigenvalue estimates on surfaces*, Math. Z. **240** (2002), no. 2, 423–449.
- [4] C. Bär, *Lower eigenvalue estimates for Dirac operators*, Math. Ann. **293** (1992), no. 1, 39–46.
- [5] M. V. Berry and R. J. Mondragon, *Neutrino billiards: time-reversal symmetry-breaking without magnetic fields*, Proc. Roy. Soc. London Ser. A **412** (1987), no. 1842, 53–74.
- [6] B. Booß-Bavnbek, M. Lesch, and Ch. Zhu, *The Calderón projection: new definition and applications*, J. Geom. Phys. **59** (2009), no. 7, 784–826.
- [7] B. Booß-Bavnbek and K. P. Wojciechowski, *Elliptic boundary problems for Dirac operators*, Mathematics: Theory & Applications, Birkhäuser Boston, Inc., Boston, MA, 1993.
- [8] H. Brezis, *Analyse fonctionnelle*, Collection Mathématiques Appliquées pour la Maîtrise., Masson, Paris, 1983, Théorie et applications. [Theory and applications].
- [9] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *The electronic properties of graphene*, Rev. Mod. Phys. **81** (2009), 109–162.
- [10] G. B. Folland, *Introduction to partial differential equations*, second ed., Princeton University Press, Princeton, NJ, 1995.
- [11] P. Freitas and P. Siegl, *Spectra of graphene nanoribbons with armchair and zigzag boundary conditions*, Rev. Math. Phys. **26** (2014), no. 10, 1450018, 32.
- [12] Th. Friedrich, *Der erste Eigenwert des Dirac-Operators einer kompakten, Riemannschen Mannigfaltigkeit nichtnegativer Skalarkrümmung*, Math. Nachr. **97** (1980), 117–146.
- [13] O. Hijazi, S. Montiel, and X. Zhang, *Eigenvalues of the Dirac operator on manifolds with boundary*, Comm. Math. Phys. **221** (2001), no. 2, 255–265.

- [14] Ch. Pommerenke, *Boundary behaviour of conformal maps*, Grundlehren der mathematischen Wissenschaften. [A Series of Comprehensive Studies in Mathematics], Springer-Verlag, Berlin Heidelberg New York, 1991.
- [15] L. A. Ponomarenko, F. Schedin, M. I. Katsnelson, R. Yang, E. W. Hill, K. S. Novoselov, and A. K. Geim, *Chaotic Dirac billiard in graphene quantum dots*, Science **320** (2008), no. 5874, 356–358.
- [16] M. Prokhorova, *The spectral flow for Dirac operators on compact planar domains with local boundary conditions*, Comm. Math. Phys. **322** (2013), no. 2, 385–414.
- [17] K. M. Schmidt, *A remark on boundary value problems for the Dirac operator*, Quart. J. Math. Oxford Ser. (2) **46** (1995), no. 184, 509–516.
- [18] E. Stockmeyer and S. Vugalter, *Infinite mass boundary conditions for Dirac operators*, To appear.

RAFAEL D. BENGURIA, EDGARDO STOCKMEYER AND HANNE VAN DEN BOSCH, INSTITUTO DE FÍSICA, PONTIFICIA UNIVERSIDAD CATÓLICA DE CHILE, VICUÑA MACKENNA 4860, SANTIAGO 7820436, CHILE.

SØREN FOURNAIS, DEPARTMENT OF MATHEMATICS, AARHUS UNIVERSITY, NY MUNKEGADE 118, DK-8000 AARHUS, DENMARK